

09831954

FILE 'HOME' ENTERED AT 14:21:22 ON 14 NOV 2002

=> file reg

COST IN U.S. DOLLARS

SINCE FILE
ENTRY

TOTAL
SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 14:21:32 ON 14 NOV 2002

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 13 NOV 2002 HIGHEST RN 473527-47-8

DICTIONARY FILE UPDATES: 13 NOV 2002 HIGHEST RN 473527-47-8

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

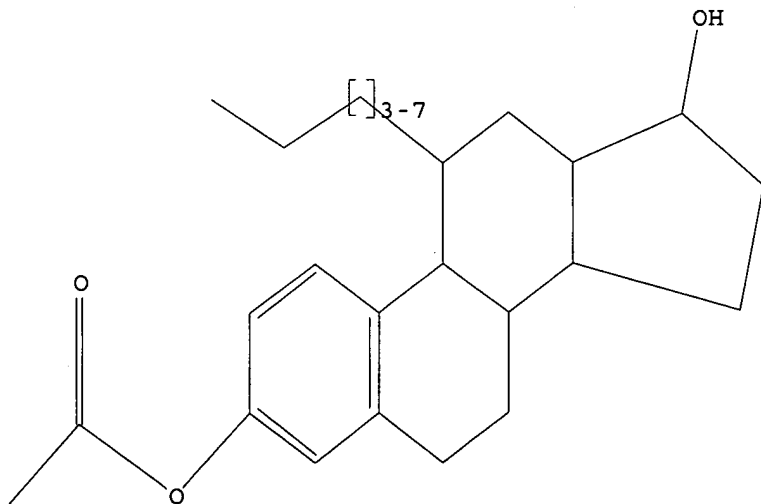
Uploading anna.str

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



steroids

09831954

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 14:22:08 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 23988 TO ITERATE

100.0% PROCESSED 23988 ITERATIONS
SEARCH TIME: 00.00.01

6 ANSWERS

L2 6 SEA SSS FUL L1

=> d 1-6

L2 ANSWER 1 OF 6 REGISTRY COPYRIGHT 2002 ACS

RN 367269-94-1 REGISTRY

CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethenyl-11-hexyl-, 3-acetate,
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 11.beta.-Hexyl-8.beta.-vinyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate

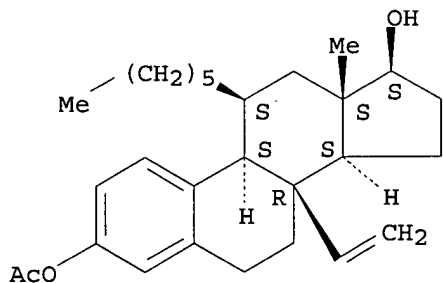
FS STEREOSEARCH

MF C28 H40 O3

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 2 OF 6 REGISTRY COPYRIGHT 2002 ACS

RN 367269-93-0 REGISTRY

CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethyl-11-hexyl-, 3-acetate,
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 8.beta.-Ethyl-11.beta.-hexyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate

FS STEREOSEARCH

MF C28 H42 O3

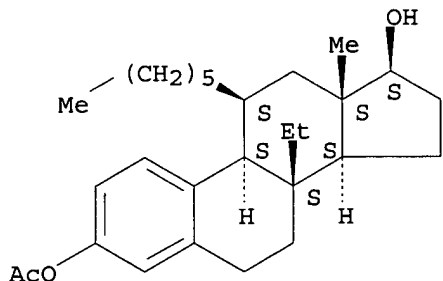
SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

steroids

09831954



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

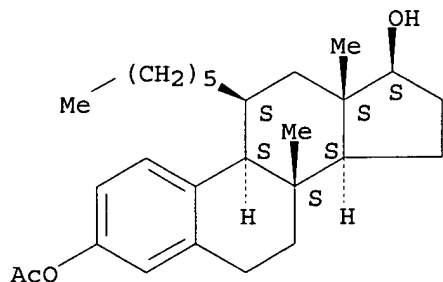
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 3 OF 6 REGISTRY COPYRIGHT 2002 ACS
RN 367269-92-9 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-hexyl-8-methyl-, 3-acetate,
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 11.beta.-Hexyl-8.beta.-methyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate
FS STEREOSEARCH
MF C27 H40 O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 4 OF 6 REGISTRY COPYRIGHT 2002 ACS
RN 367269-91-8 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethenyl-11-pentyl-, 3-acetate,
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

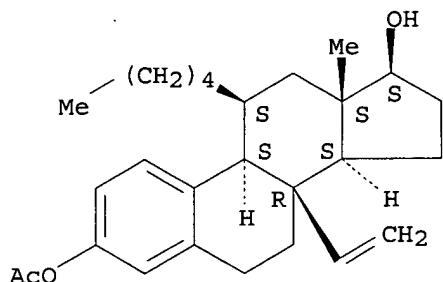
OTHER NAMES:

CN 11.beta.-Pentyl-8.beta.-vinyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate
FS STEREOSEARCH
MF C27 H38 O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

steroids

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Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

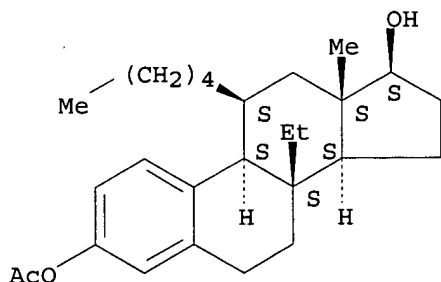
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 5 OF 6 REGISTRY COPYRIGHT 2002 ACS
RN 367269-90-7 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethyl-11-pentyl-, 3-acetate,
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 8.beta.-Ethyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate
FS STEREOSEARCH
MF C27 H40 O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 6 OF 6 REGISTRY COPYRIGHT 2002 ACS
RN 367269-89-4 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 8-methyl-11-pentyl-, 3-acetate,
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

OTHER NAMES:

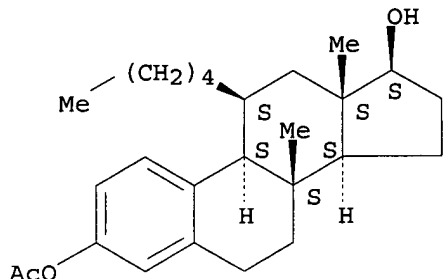
CN 8.beta.-Methyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate
FS STEREOSEARCH

steroids

09831954

MF C26 H38 O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> file ca caplus
COST IN U.S. DOLLARS
FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
150.14	150.35

FILE 'CA' ENTERED AT 14:22:31 ON 14 NOV 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE 'CAPLUS' ENTERED AT 14:22:31 ON 14 NOV 2002
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COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

=> s l2
L3 2 L2

=> d 1-2 .mano hitstr

L3 ANSWER 1 OF 2 CA COPYRIGHT 2002 ACS
TI Preparation of 8.beta.-substituted-11.beta.-pentyl- and
11.beta.-hexyl-estra-1,3,5(10)-triene derivatives which have an affinity
for the estrogen receptor
SO PCT Int. Appl., 53 pp.
CODEN: PIXXD2
AB The present invention relates to the novel 8.beta.-substituted
estra-1,3,5(10)-trienes I [R2 = H, F, Cl, Br, I, straight or branched
(un)satd. C1-6-alkyl, OH, alkoxy, acyloxy, CF3, sulfamoyloxy; R3 = alkoxy,
sulfamoyloxy, acyloxy; R6, R6' = H; R6R7 = bond; R7, R7' = H ; R8 means a
straight-chain or branched-chain, optionally partially or entirely
halogenated alkyl or alkenyl radical having up to 5 carbon atoms, an
ethynyl or prop-1-ynyl radical; R11 = pentyl, hexyl; R14 = H; R14R15 =
bond ; R15 = H; R15', R16' = H, F, Cl, Br, I, alkoxy, sulfamoyloxy,

steroids

acyloxy; R15R16 = bond; R16 = H; R17, R17' = H, H and halogen, H and OCH2Ph, H and sulfamoyloxy; alkyl and acyl or acyloxy; alkoxy and alkyl, alkoxy and acyloxy; R17R17' = CH2 CR23R24; R23, R24 = H, halogen; R23R24 = O]. Thus, 8.beta.-methyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol (II) was prepd. from 8.beta.-cyanosteroid III (R25 = CN) via condensation of 11-ketosteroid III (R25 = Me) with BuCH2Li. Estradienes I are used as pharmaceutical active agents which, in vitro, are provided with a higher affinity of estrogen receptor prepsns. of rat prostate than of estrogen receptor prepsns. of rat uterus and, in vivo, preferably act in a preferential contraceptive manner on the ovary without stimulating the uterus. The invention also relates to the prodn. thereof, the therapeutic use thereof and pharmaceutical administration forms which contain the novel compds. I. The invention further relates to the use of compds. I for male contraception and to the use of non-malignant or malignant proliferate diseases of the ovary, such as ovarian carcinoma or granulosa cell tumors for instance.

PY 2001
2001

IN Peters, Olaf; Braeuer, Nico; Hillisch, Alexander; Hegele-Hartung, Christa; Fritzemeier, Karl-Heinrich

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001077138	A1	20011018	WO 2001-EP4289	20010412

PI DE 10019167 A1 20011018 DE 2000-10019167 20000412

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CO, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, 'KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

IT 367269-89-4P, 8.beta.-Methyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-90-7P, 8.beta.-Ethyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-91-8P, 11.beta.-Pentyl-8.beta.-vinyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-92-9P, 11.beta.-Hexyl-8.beta.-methyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-93-0P, 8.beta.-Ethyl-11.beta.-hexyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-94-1P, 11.beta.-Hexyl-8.beta.-vinyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

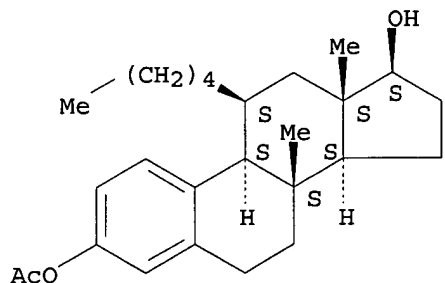
(prepn. of 8.beta.-substituted-11.beta.-pentyl- and -11.beta.-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the estrogen receptor)

RN 367269-89-4 CA

CN Estra-1,3,5(10)-triene-3,17-diol, 8-methyl-11-pentyl-, 3-acetate, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

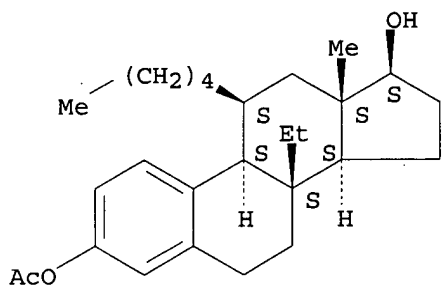
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RN 367269-90-7 CA

CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethyl-11-pentyl-, 3-acetate,
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

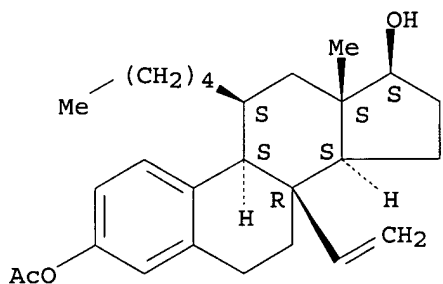
Absolute stereochemistry.



RN 367269-91-8 CA

CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethenyl-11-pentyl-, 3-acetate,
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



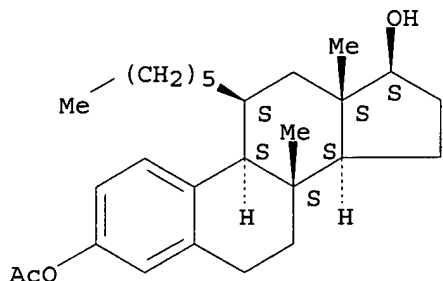
RN 367269-92-9 CA

CN Estra-1,3,5(10)-triene-3,17-diol, 11-hexyl-8-methyl-, 3-acetate,
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

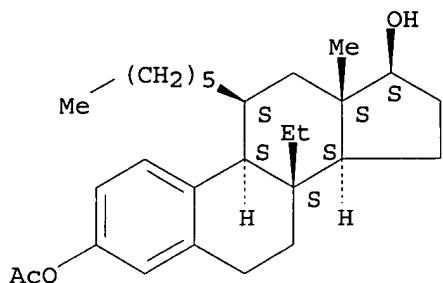
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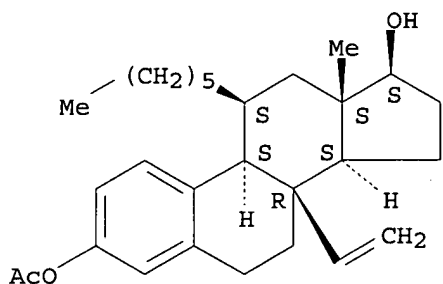
RN 367269-93-0 CA
CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethyl-11-hexyl-, 3-acetate,
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 367269-94-1 CA
CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethenyl-11-hexyl-, 3-acetate,
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS
TI Preparation of 8.beta.-substituted-11.beta.-pentyl- and
11.beta.-hexyl-estra-1,3,5(10)-triene derivatives which have an affinity
for the estrogen receptor
SO PCT Int. Appl., 53 pp.
CODEN: PIXXD2
AB The present invention relates to the novel 8.beta.-substituted
estra-1,3,5(10)-trienes I [R₂ = H, F, Cl, Br, I, straight or branched
(un)satd. C1-6-alkyl, OH, alkoxy, acyloxy, CF₃, sulfamoyloxy; R₃ = alkoxy,
sulfamoyloxy, acyloxy; R₆, R₆' = H; R₆R₇ = bond; R₇, R₇' = H ; R₈ means a

steroids

straight-chain or branched-chain, optionally partially or entirely halogenated alkyl or alkenyl radical having up to 5 carbon atoms, an ethynyl or prop-1-ynyl radical; R11 = pentyl, hexyl; R14 = H; R14R15 = bond; R15 = H; R15', R16' = H, F, Cl, Br, I, alkoxy, sulfamoyloxy, acyloxy; R15R16 = bond; R16 = H; R17, R17' = H, H and halogen, H and OCH2Ph, H and sulfamoyloxy; alkyl and acyl or acyloxy; alkoxy and alkyl, alkoxy and acyloxy; R17R17' = CH2 CR23R24; R23, R24 = H, halogen; R23R24 = O]. Thus, 8.beta.-methyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol (II) was prepd. from 8.beta.-cyanosteroid III (R25 = CN) via condensation of 11-ketosteroid III (R25 = Me) with BuCH2Li. Estradienes I are used as pharmaceutical active agents which, in vitro, are provided with a higher affinity of estrogen receptor preps. of rat prostate than of estrogen receptor preps. of rat uterus and, in vivo, preferably act in a preferential contraceptive manner on the ovary without stimulating the uterus. The invention also relates to the prodn. thereof, the therapeutic use thereof and pharmaceutical administration forms which contain the novel compds. I. The invention further relates to the use of compds. I for male contraception and to the use of non-malignant or malignant proliferate diseases of the ovary, such as ovarian carcinoma or granulosa cell tumors for instance.

PY 2001

2001

IN Peters, Olaf; Braeuer, Nico; Hillisch, Alexander; Hegele-Hartung, Christa; Fritzemeier, Karl-Heinrich

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	WO 2001077138	A1	20011018	WO 2001-EP4289	20010412
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W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CO, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

DE 10019167	A1	20011018	DE 2000-10019167	20000412
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IT 367269-89-4P, 8.beta.-Methyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-90-7P, 8.beta.-Ethyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-91-8P, 11.beta.-Pentyl-8.beta.-vinyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-92-9P, 11.beta.-Hexyl-8.beta.-methyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-93-0P, 8.beta.-Ethyl-11.beta.-hexyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-94-1P, 11.beta.-Hexyl-8.beta.-vinyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 8.beta.-substituted-11.beta.-pentyl- and -11.beta.-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the estrogen receptor)

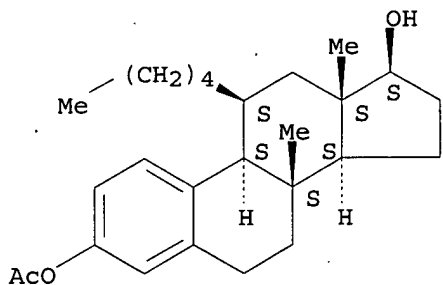
RN 367269-89-4 CAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 8-methyl-11-pentyl-, 3-acetate, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

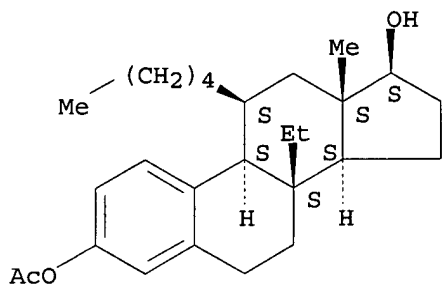
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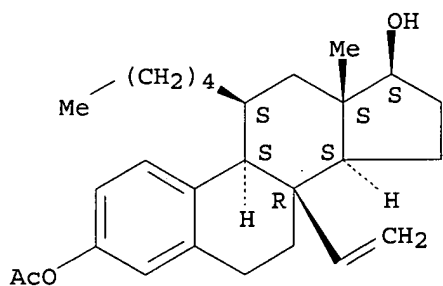
RN 367269-90-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethyl-11-pentyl-, 3-acetate,
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 367269-91-8 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethenyl-11-pentyl-, 3-acetate,
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

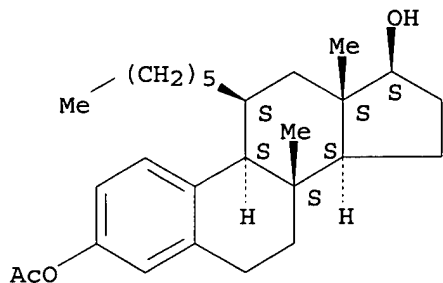


RN 367269-92-9 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-hexyl-8-methyl-, 3-acetate,
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

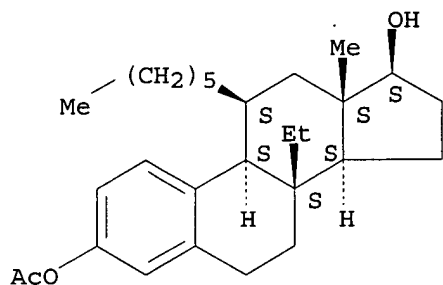
steroids

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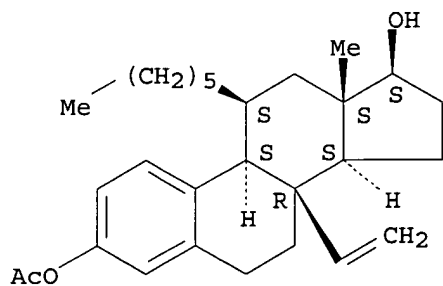
RN 367269-93-0 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethyl-11-hexyl-, 3-acetate,
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 367269-94-1 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethenyl-11-hexyl-, 3-acetate,
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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steroids